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The focus of the program is the development and application of an algorithm for studying charge transport in low temperature gallium arsenide (LT GaAs) buffer layers and the influence of such layers on device operation. During this reporting period the drift and diffusion equations were modified to include the contributions of clusters in one and two dimensions. In addition, the *effects* of high resistance material on the operation of FETs was begun. Specifically numerical simulations of clusters in LT GaAs were performed in which the electrical characteristics of the clusters were modeled as local trap sites. Simulations were performed for a single cluster in one dimension, two clusters in one dimension, and an array of clusters in two dimensions. The one-dimensional simulations of a single cluster demonstrate the depletion of mobile charge around the cluster and barrier-like electrostatic behavior. Double cluster simulations, also in one dimension, show the effect of overlapping depletion regions. Two-dimensional simulations of arrays of clusters show how the interaction between the clusters results in an insulating material. Finally, a macroscopic model of the LT material is utilized in the simulation of an FET with an LT layer under the gate. The results suggest that such structures should have enhanced breakdown characteristics without adversely affecting performance. (Interaction with Wright Laboratories and Lincoln Laboratories on organization of an APS-focused session on LTR materials and future directions is also summarized.

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For

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Bolling Air Force Base
Washington, DC 20332-6448

April 1993

Numerical Studies of Low Temperature Gallium Arsenide Buffer Layers and Their Influence on Device Operation

Annual Report

Introduction

The focus of the program is the development and application of an algorithm for studying charge transport in low temperature gallium arsenide (LT GaAs) buffer layers and the influence of such layers on device operation. During this reporting period the drift and diffusion equations were modified to include the contributions of clusters in one and two dimensions. In addition, the *effects* of high resistance material on the operation of FETs was begun. Specifically numerical simulations of clusters in LT GaAs were performed in which the electrical characteristics of the clusters were modeled as local trap sites. Simulations were performed for a single cluster in one dimension, two clusters in one dimension, and an array of clusters in two dimensions. The one-dimensional simulations of a single cluster demonstrate the depletion of mobile charge around the cluster and barrier-like electrostatic behavior. Double cluster simulations, also in one dimension, show the effect of overlapping depletion regions. Two-dimensional simulations of arrays of clusters show how the interaction between the clusters results in an insulating material. Finally, a macroscopic model of the LT material is utilized in the simulation of an FET with an LT layer under the gate. The results suggest that such structures should have enhanced breakdown characteristics without adversely affecting performance.

The Model

The present model is based on the continuity equations, including generation and recombination

$$\frac{\partial n}{\partial t} = \frac{1}{e} \nabla \bullet J_n + G_n - R_n \qquad (1)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{e}\nabla \bullet J_p + G_p - R_p \qquad (2)$$

which identify local time dependent changes in electron n, and hole, p, carrier density. J_n and J_p represent the current density of electrons and holes. G and R represent the net generation and recombination that include capture and emission of electrons and holes by deep level trapping centers.

The kinetics of capture and emission from donors and acceptors determine the recombination rates for electrons, R_n and holes, R_p introduced into equations (1) and (2).

$$G_n - R_n = C_n^-\left[n_1^a N_A^- - n N_A^o\right] + C_n^+\left[n_1^d N_D^o - n N_D^+\right] \qquad (3)$$

where C_n^+ and C_n denote capture rate of electrons from acceptors and donors, respectively. For holes the net recombination rate is:

$$G_p - R_p = C_p^-\left[p_1^a N_A^o - p N_A^-\right] + C_p\left[p_1^d N_D^+ - p N_D^o\right] \qquad (4)$$

where C_p^- and C_p denote capture rates of holes from acceptors and donors, respectively. The n_1 and p_1 terms are obtained from equilibrium conditions, and under nondegenerate conditions are approximated by the equations:

$$n_1^a = N_c \exp -\left[\left(E_c - E_a\right) / k_B T\right], \quad n_1^d = N_c \exp -\left[\left(E_c - E_d\right) / k_B T\right] \qquad (5)$$

$$p_1^a = N_v \exp -\left[\left(E_a - E_v\right) / k_B T\right], \quad p_1^d = N_v \exp -\left[\left(E_d - E_v\right) / k_B T\right] \qquad (6)$$

The filling and emptying of the donor and acceptor states occurs during a finite time period and is governed by the same kinetics as discussed above. For a single acceptor level and a single donor level the rate of change of the population of these levels is given by

$$\frac{\partial N_A^-}{\partial t} = C_p^-\left[p_1^a N_A^o - p N_A^-\right] + C_n\left[n N_A^o - n_1^a N_A^-\right] \qquad (7)$$

$$\frac{\partial N_D^+}{\partial t} = c_n^+\left[n_1^d N_D^o - n N_D^+\right] + c_p\left[p N_D^o - p_1^d N_D^+\right] \quad (8)$$

The above equations (1), (2), (7), and (8) identify several components of the continuity equation. The constitutive relationships for current density are given below:

$$J_n = -e\left[n\mu_n \nabla\psi - D_n \nabla n\right] \quad (9)$$

$$J_p = -e\left[p\mu_p \nabla\psi + D_p \nabla p\right] \quad (10)$$

Finally, Poisson's equation is introduced as

$$\nabla \bullet \epsilon \nabla\psi = e(n - p - \langle c \rangle) \quad (11)$$

where $\langle c \rangle$ s the net concentration of ionized donors and acceptors arising from both deep level traps as well as shallow dopants. In the present model, the deep level traps represent the As clusters whereas the shallow, fully ionized dopants represent the doping level of the surrounding GaAs material.

Results

One-Dimensional Simulation

Single Cluster

The first simulations performed were for a single cluster. The structure considered was representative of a cluster 100Å in diameter surrounded by material doped to various levels. Both N and P type material was considered. The ratio of deep level donors to acceptors was varied. For $N_D/N_A = 1.014$, $(E_c - E_f) = 0.8$eV in the cluster. All results showed similar behavior. The mobile electrons (holes) surrounding the cluster would diffuse into the cluster and neutralize deep level donors (acceptors). The region surrounding the cluster is depleted of mobile charge and a potential distribution similar to that at a Schottky barrier is established. The height of the potential barrier is dependent on the density of the shallow dopants surrounding the cluster since the kinetics of the cluster determined the electron density within the cluster. An example of such a result is

given in Figs. 1-3 where the potential, electron concentration and space charge are given for the case of $(E_c - E_f) = 0.8$ and shallow donors at $1x10^{17}/cm^3$.

Dual Cluster

The second series of simulations performed was for a structure representing two clusters separated by 200Å. These simulations were also performed for a range of shallow dopant densities. For doping levels below $10^{18}/cm^3$ (N or P type), the region between the clusters was completely depleted and the material would have an insulating nature. As the doping level exceeded $10^{18}/cm^3$, the clusters were unable to fully deplete the surrounding material and the insulating properties are reduced. This result is consistent with the conclusions of Ref. 1. It should be recognized, however, that the exact limits of where significant conduction would begin to occur, would depend on the trap kinetics and deep level densities specified in the model . An example of the potential, electron and space charge distribution between the two clusters is shown in Figs. 4-6, again for $(E_c - E_f) = 0.8$ and shallow donors of $4x10^{18}/cm^3$ where the material is just beginning to exhibit conductive properties.

Two-Dimensional Simulation

The third simulations of discrete clusters involves two-dimensional arrays of clusters. Here, clusters 75Å in diameter are separated by 125Å. Two rows of clusters were considered. In one case the clusters in the two rows are aligned such that four clusters, two from each row, formed the corners of a square. In the second case the clusters are staggered such that three clusters create a triangle. Such simulations are useful in studying material properties and characteristics.

Aligned Clusters

Three aligned clusters simulations were performed at bias levels of 0.0, 0.5 and 1.0 volts across 600 Å of material doped to $1x10^{18}/cm^3$. The results all showed depletion of the material surrounding the clusters rendering the material highly sensitive. At a bias level of 1.0 volts a very low current began to flow. Contour plots of the electron density and potential for this case are shown in Figs. 7 and 8. In Fig. 7 we observe fingers of charge extending between the clusters which are created by the injection of electrons from

the cathode under the influence of the applied bias. Even with this high average field, which exceeds 150 kV/cm, the highest electron density between the clusters is only of the order of $1x10^{14}/cm^3$. Figure 8 shows the corresponding distribution of potential. Here we note the high field region on the anode side of the device.

Staggered Clusters

Typical results for a staggered cluster arrangement are shown in Figs. 9-10 at a bias of 0.5 volts. Here the bulk material is again $10^{18}/cm^3$ N type. In Fig. 9 the contours of electron density show that in the insulating region between the clusters the electron density is below $1x10^{10}/cm^3$. The initiation of charge injection into the insulating material is apparent, however not yet significant. Contours of potential are shown in Fig. 10. The overlapping depletion regions with a minimum potential of –0.65 volts at the center of the cathode side clusters can be observed. A high field region on the anode side is also present. No current has begun to flow yet.

FET Simulation

The final simulations considered are for a full device structure. In this simulation a microscopic model of the clusters in LT GaAs was not used. The study addresses only the effect of the high resistance region on the electrical characteristics of the FET. For this calculation the same set of rate equations described at the beginning of this paper was used. Thus, in the macroscopic model a uniform continuous distribution of traps is used in regions of LT material. Based on the density and size of clusters a nominal trap density of the order of $1x10^{18}/cm^3$ in the LT material follows. Simulations of a FET, with and without a LT buffer layer under the gate showed that the use of a thin buffer layer could enhance the breakdown characteristics of the device without adversely effecting performance. For the structure considered, a 0.5μm gate FET with 2.5μm source-drain spacing, the transconductance and cut-off frequency were only slightly effected by the presence of a 200Å thick LT gate buffer layer. The major negative effect was an increase in the threshold voltage from -1.12 volts to -1.95 volts. However, the current path avoids the high field region near the gate and breakdown should be delayed.

Future Studies

Future studies will include a more complete analysis of the two-dimensional cluster

model. These studies will include the placement of clusters within heterostructure regions. In addition, attempts will be made to include the effects of clusters in the FET model, although here we recognize that the limitations of machine space may force us to deal with a somewhat abbreviated model. Additionally, we intend to collaborate with Lincoln Laboratories and model the electrical characteristics of select structures such as N(LT)N structures for detailed comparison with experiments.

Presentations, Publications and Interactions

The PI of this project, along with J. Woodall, organized a focussed session on LTG materials at the March Meeting of the American Physical Society. In addition, an invited paper on LTG materials was presented at this meeting.

The results of the LTG studies were presented at the 1993 WOCSEMMAD.

The LTG results and a brief discussion of reliability studies was undertaken by the PI on a visit to Wright Laboratories. Additionally, a collaboration on the LT studies with Lincoln Laboratories has been initiated.

A detailed paper on the simulations and the trap model of clusters is being prepared for submission to the Journal of Applied Physics.

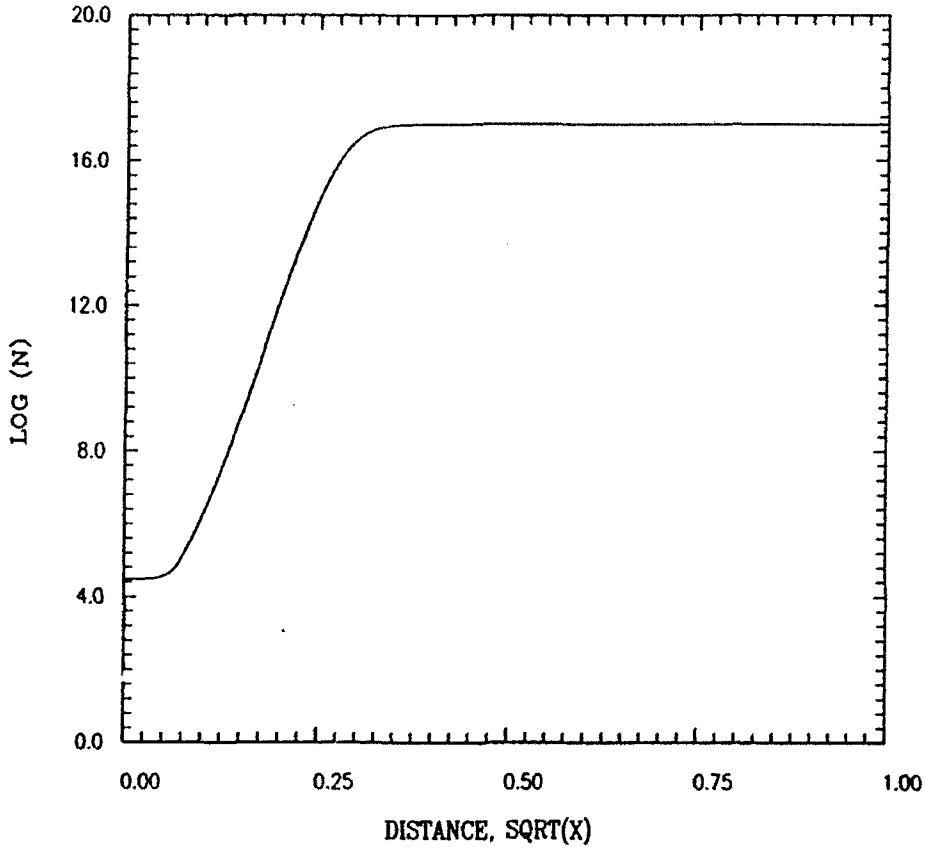

Figure 1. Density distribution surrounding a single cluster for a shallow dopant level of $1x10^{17}/cm^3$. Cluster ends at $x^{1/4} = .07071$.

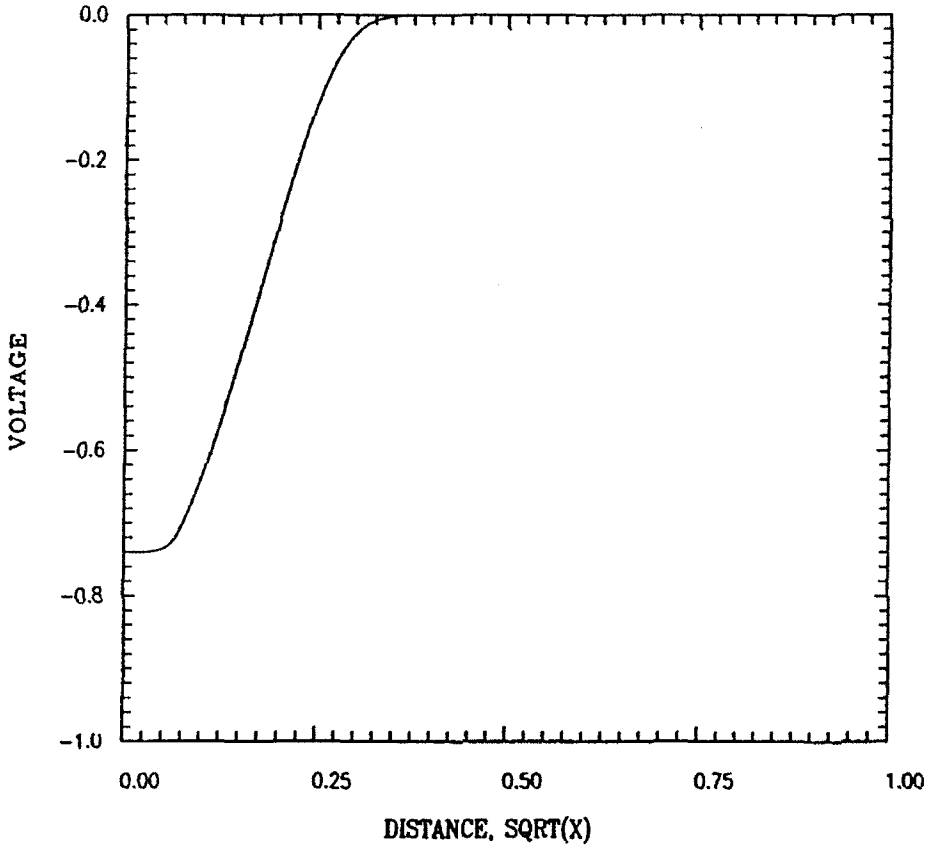

Figure 2. Potential distribution surrounding a single cluster.

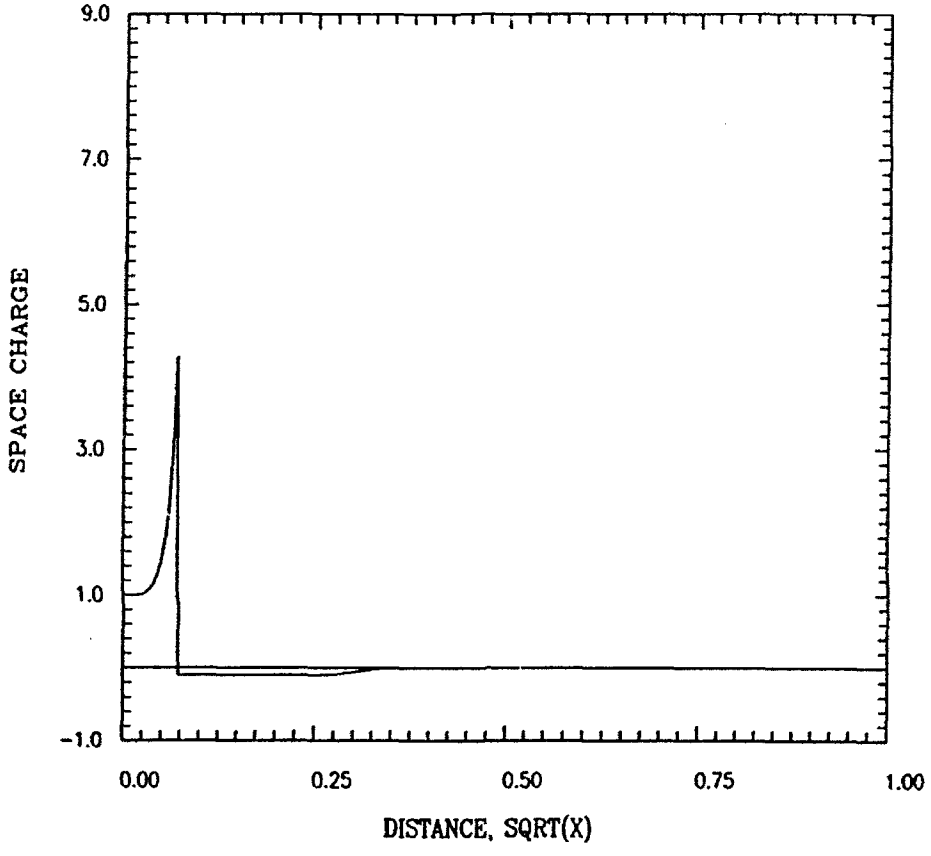

Figure 3. Normalized space charge distribution surrounding a single cluster, $\rho = (n - p - N_{D_S} + N_{A_S} - N_D^+ + N_A^-)/(1x10^{18}/cm^3)$.

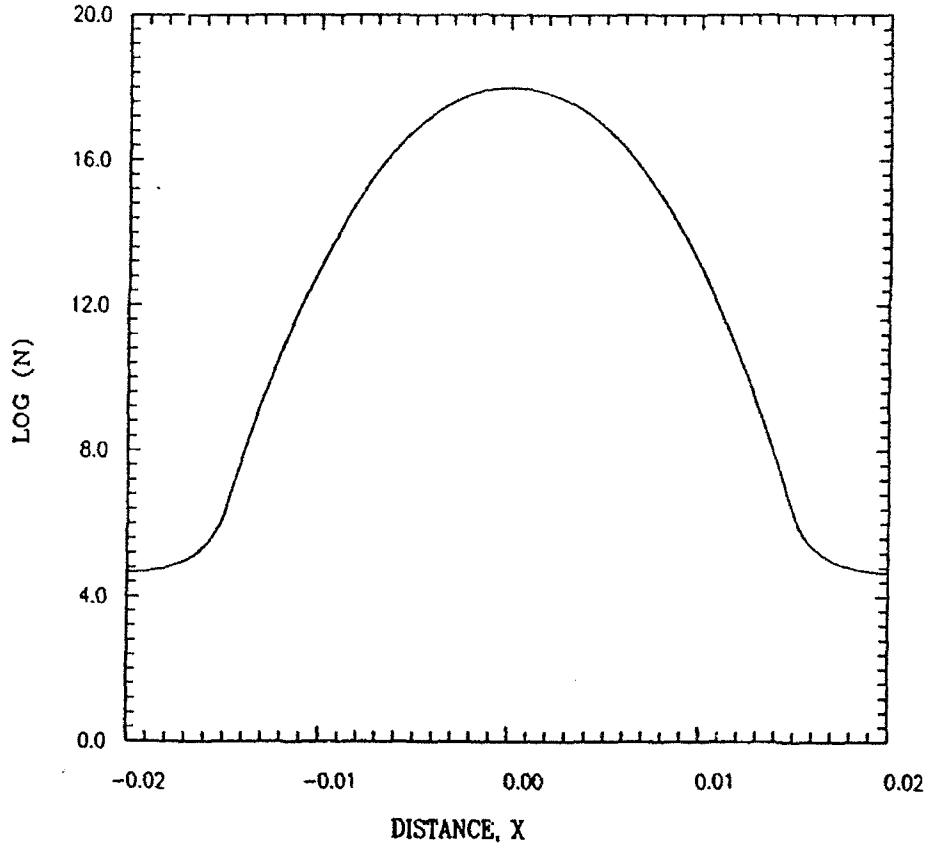

Figure 4. Density distribution between two clusters for a shallow dopant density of $4x10^{18}/cm^3$.

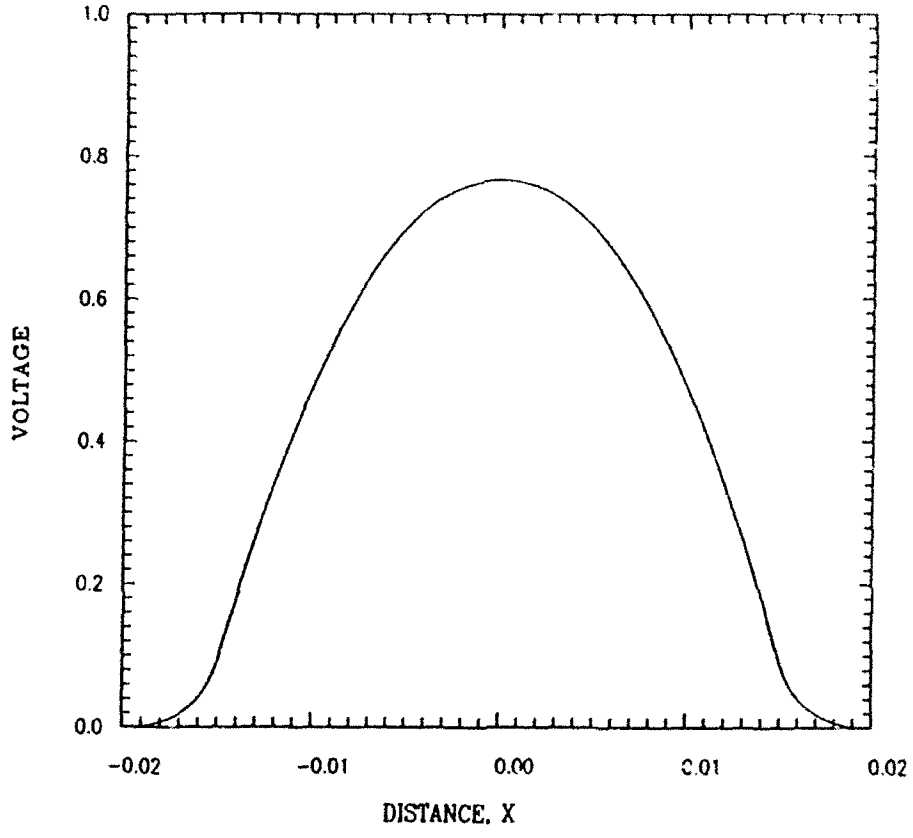

Figure 5. Potential distribution between two clusters for a shallow dopant density of $4x10^{18}/cm^3$.

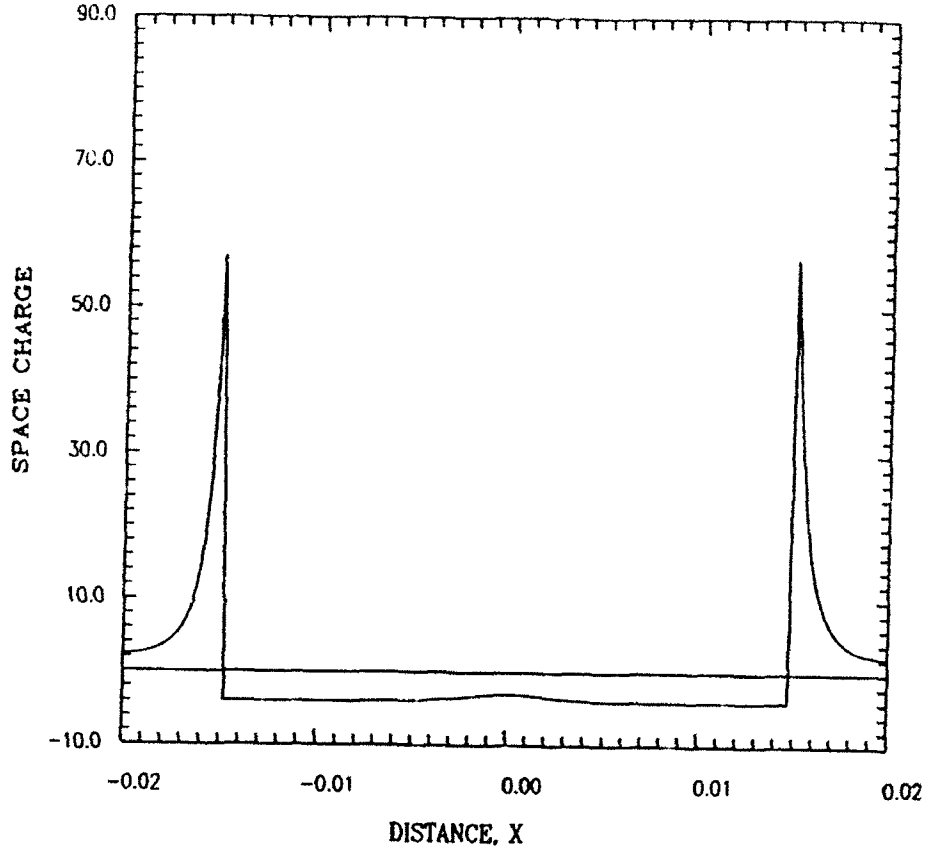

Figure 6. Normalized space charge distribution between two clusters, $\rho = (n - p - N_{D_S} + N_{A_S} - N_D^+ + N_A^-)/(1x10^{18}/cm^3)$.

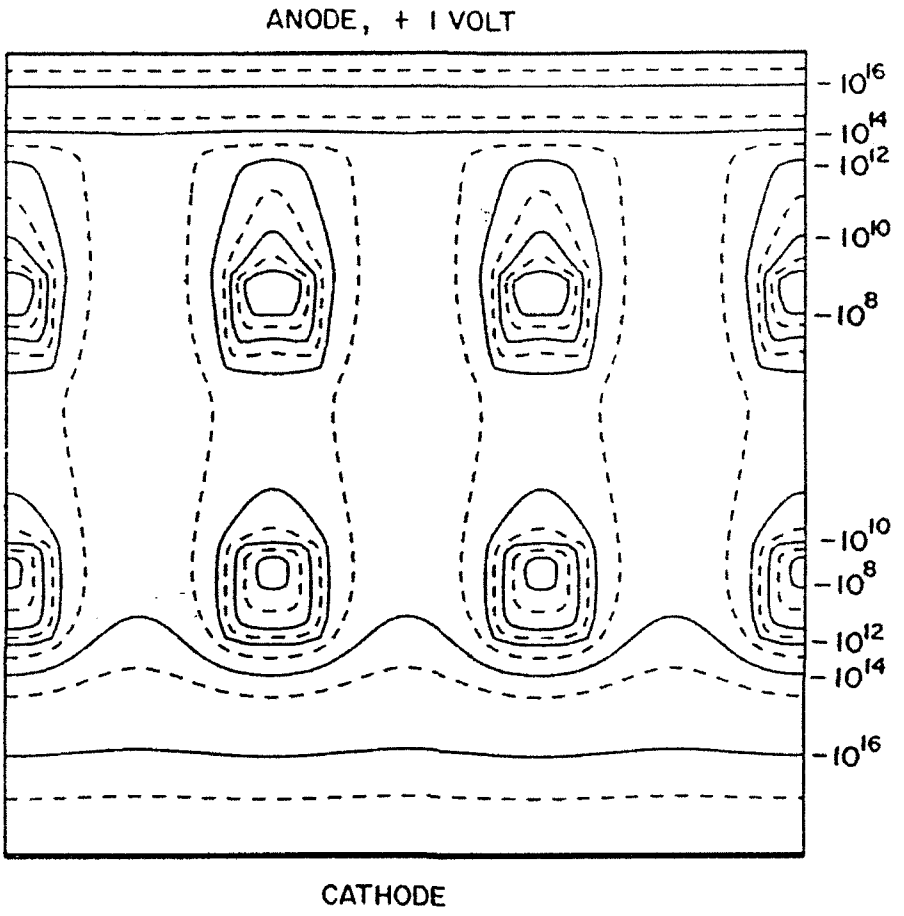

Figure 7. Density distribution surrounding an array of clusters with 1.0 volts bias. Opening level is $1x10^{18}/cm^3$.

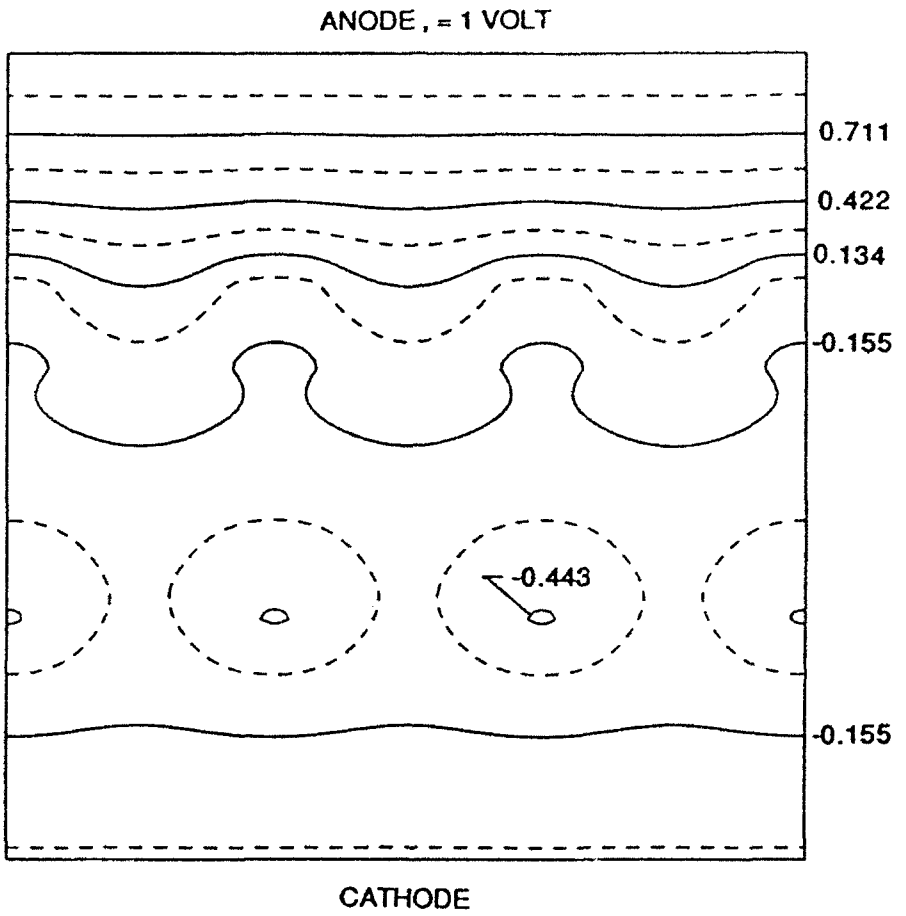

Figure 8. Potential distribution surrounding an array of clusters with a bias of 1.0 volts. Doping level is $1x10^{18}/cm^3$.

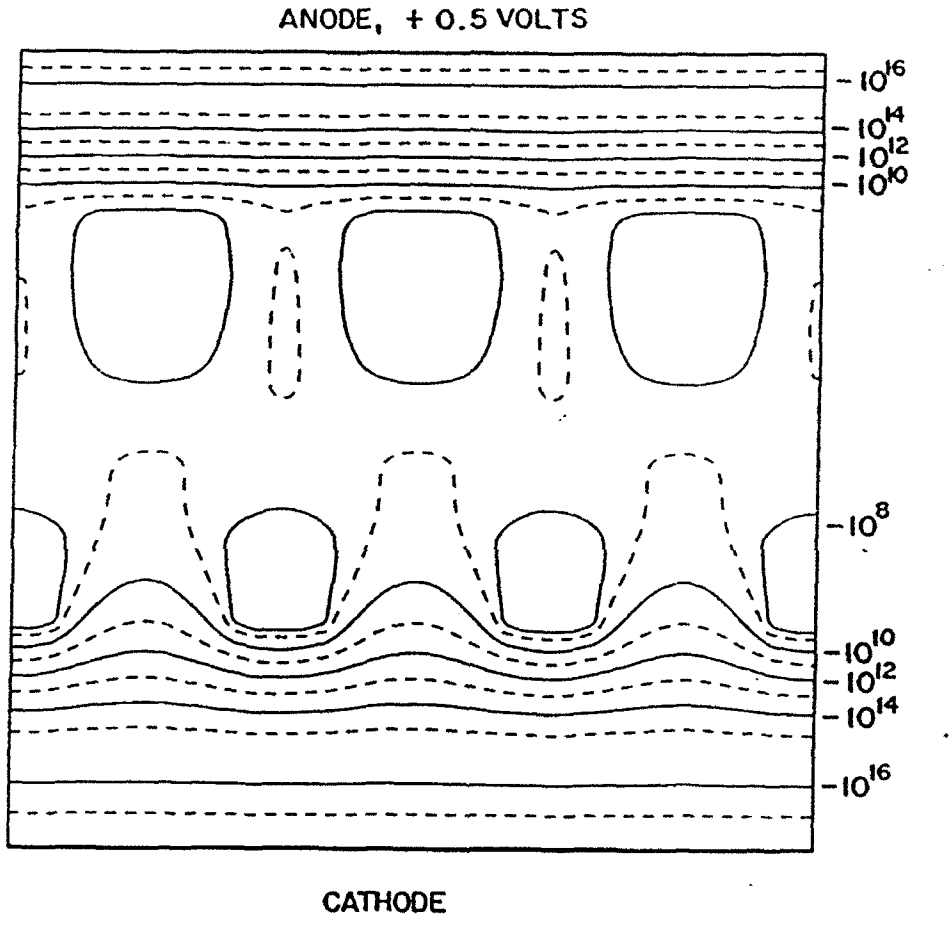

Figure 9. Density distribution surrounding an array of clusters with 0.5 volts bias. Opening level is $1x10^{18}/cm^3$.

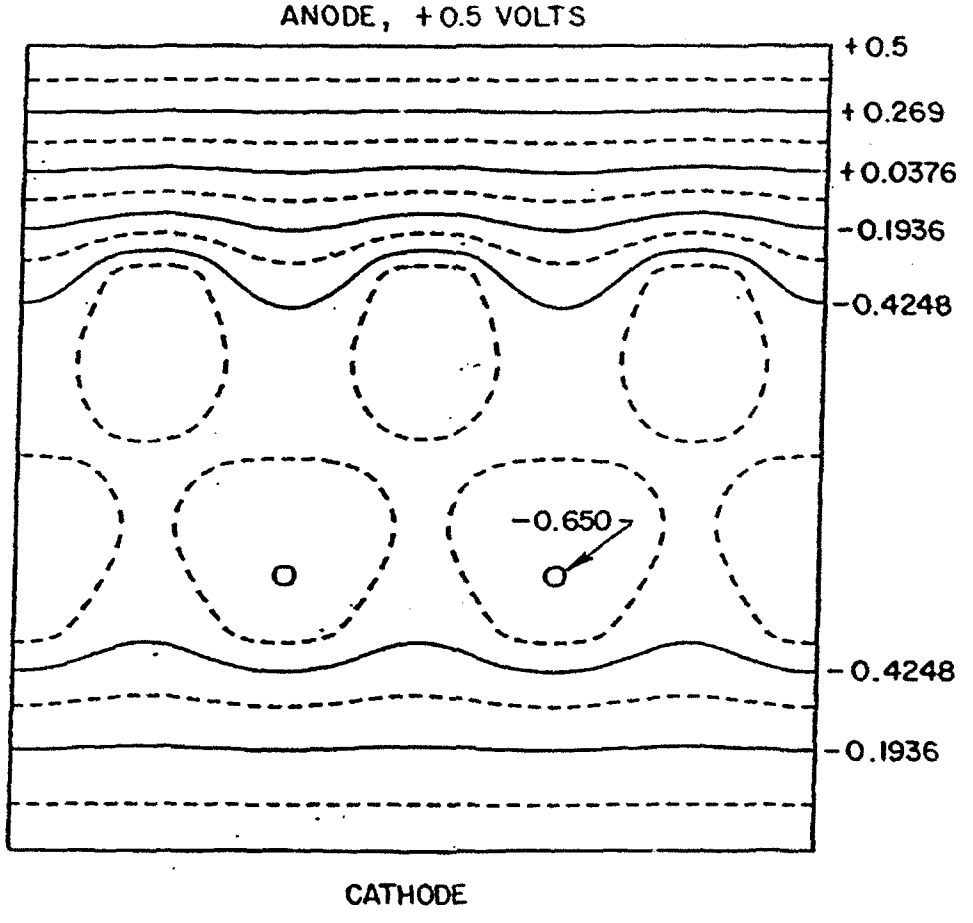

Figure 10. Potential distribution surrounding an array of clusters with a bias of 0.5 volts. Doping level is $1x10^{18}/cm^3$.